Spin correlations and phase diagram of the perturbed Kitaev model

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We present a general classification of the perturbations to the Kitaev model on the basis of their effect on it's spin correlation functions. We derive a necessary and sufficient condition for the spin correlators to exhibit a long ranged power-law behavior in the presence of such perturbations. We substantiate our result by a study of the phase diagram of the Kitaev model augmented by a loop term and perturbed by an Ising term, within a RVB mean-field theory. We estimate the stability of the spin-liquid phase against such perturbations and show that this model exhibits both confinement-deconfinement transitions from spin liquid to antiferromagnetic/spin-chain/ferromagnetic phases as well as topological quantum phase transitions between gapped and gapless spin liquid phases.

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The spin-1/2 Kitaev model on a honeycomb lattice (Fig 1), a rare example of an exactly solvable 2D quantum spin model, is known to have several interesting features [1–4]. The Hamiltonian for the model is given by

$$H_K = \sum_{j+l=\text{even}} (J_1\sigma^x_{j,l}\sigma^x_{j+1,l} + J_2\sigma^y_{j-1,l}\sigma^y_{j,l} + J_3\sigma^z_{j,l}\sigma^z_{j,l+1}), \quad (1)$$

where j and l denote the column and row indices of the lattice and $\sigma^{x,y,z}$ are Pauli matrices. The model has spin liquid ground states and exhibits spin fractionalization at all energy scales with extremely short ranged (nearest neighbour) spin-spin correlations [3]. The spectrum is gapless for $|J_1 - J_2| \leq J_3 \leq J_1 + J_2$ [1] and gapped otherwise. The gapped phase has Abelian anyonic excitations while the gapless phase supports non-Abelian anyons which could provide topologically protected subspaces for fault tolerant quantum computation [1, 7].

There have been several proposals for experimentally realizing this model in systems of ultracold atoms and molecules trapped in optical lattices, quantum circuits [5] and in layered iridates [6]. Almost inevitably such realizations will have contaminating perturbations; therefore the effect of such perturbation on the spin-liquid phases of the Kitaev model deserves theoretical attention. Recently, the effect of one such perturbation, namely a Zeeman field given by the Hamiltonian $H_z = -h\sum_i \sigma^z_i$, on the spin correlations of the model has been studied [8]. It was found that such a perturbation (arbitrarily weak) qualitatively alters the nature of the spin correlators by rendering them long-ranged (in power-law sense). However, such an analysis has not been extended to other relevant perturbations. In particular, there is no general theoretical criteria to classify the perturbations according to their effect on the spin correlations. Furthermore, the stability of the Kitaev spin-liquid in the presence of perturbations and the possible transitions of this perturbed Kitaev model from the deconfined spin-liquid state to the confined spin-ordered states has not been studied.

In this letter, we study both the above-mentioned issues. First, we provide an explicit classification of different short-range perturbations, in the gapless spin liquid phase, based on the nature of the spin correlators they induce. We derive the necessary and sufficient condition for the spin correlators to exhibit a long ranged power-law behavior in the presence of such perturbations and show that the induction of a long-range spin-correlation by a magnetic field, studied in Ref. [8], constitutes *a specific example* of this general condition. Following this we take up a concrete example of the second class of perturbation which does not induce long-range correlations and study the Kitaev model in the presence of a loop term and the Ising-like perturbative term . We analyze this model using a RVB mean-field approach and demonstrate that the model exhibits transitions from a deconfined spin liquid to confined Ising ordered antiferromagnetic (AFM), ferromagnetic (FM) or spin-chain (SC) phases. We also show that the model supports two distinct spin liquid phases with gapped and gapless deconfined spinon excitations with a topological quantum phase transition separating them. We chart out the phase diagram of this model and estimate the stability of the deconfined phases as a function of the strengths of the loop and Ising terms. Both the issues studied here are highly experimentally relevant and our work constitutes a significant extension of our understanding of the perturbed Kitaev model.

We begin with the study of the fate of spin correlations of the Kitaev model under most general class of short ranged perturbations. The total Hamiltonian is then given by $H = H_K + H_P$, where H_P is a perturbing Hamiltonian made up of spin operators. Examples of H_P include H_z or the most general bilinear spin-spin interaction term given by $H_b = \sum_{\langle ij\rangle} \lambda_{\alpha\beta}\sigma^\alpha_i\sigma^\beta_j$ including the experimentally most relevant anisotropic Heisenberg interaction $H_h = \sum_{\langle ij\rangle}\left(\lambda_{xx}\sigma^x_i\sigma^x_j + \lambda_{yy}\sigma^y_i\sigma^y_j + \lambda_{zz}\sigma^z_i\sigma^z_j\right)$.

In the analysis of the effects of these perturbations a crucial role is played by the Z_2 flux operators defined as

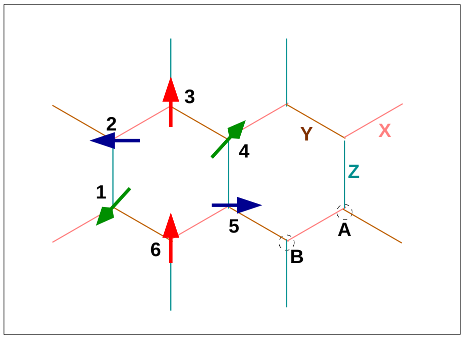

FIG. 1: (Color online) Schematic representation of the Kitaev model on a honeycomb lattice showings the different links x, y and z and the two sublattices A and B. The sites labeled 1..6 and their spin configuration is a schematic representation for a classical configuration with $\langle W_p \rangle = 1$ where the green, blue and red spins point in the x, y and z directions respectively.

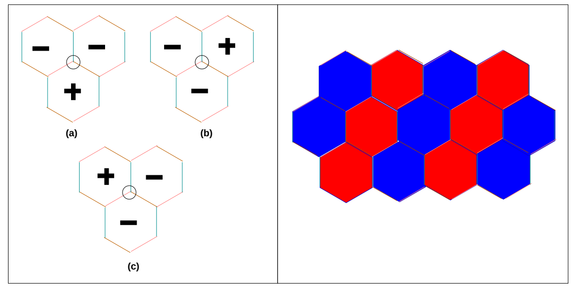

FIG. 2: (color online) Left Panel: The flux flipped on application of σ_i^α where i is the site at the center (circled): (a) $\alpha = z$, (b) $\alpha = y$ (c) $\alpha = x$ (see Fig. 1 for definition of the x, y, z bonds). Right Panel: A schematic representation of y type covering Γ_{yR} (red plaquettes) and Γ_{yB} (blue plaquettes). A product of W_p over red or blue plaquettes yields Σ^y. Analogous coverings for x and z type coverings may be obtained by rotating the above figure by $\pm 60°$

$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$ (Fig. 1) on every plaquette. Since $[H_K, W_p] = 0$ these fluxes are frozen in the unperturbed model and this fact is crucial to the integrability of the unperturbed Kitaev Model. For the ground state of H_K, $W_p = 1\ \forall p$. However, H_P does not commute with the W_ps and thus the Z_2 fluxes acquires dynamics in the perturbed model. The effect of this dynamics is key to determining the nature of the spin correlators of the perturbed Kitaev model. To this end we define 3 conserved operators, $\Sigma^\alpha \equiv \prod_j (i\sigma_j^\alpha) = \prod_{p\in\Gamma_{\alpha c}} W_p$ where $\alpha = x, y, z$ and the product over W_ps in the second expression is taken over a subset of plaquettes $\Gamma_{\alpha c}$ in the following way. Colour all the plaquettes with two colours, red and blue, as shown in Fig. 2 (right panel). Then $\Gamma_{yR}(\Gamma_{yB})$ denotes product of all W_ps on the red(blue) plaquettes which gives Σ^y. Analogous coverings in the other two directions yields Σ^x and Σ^z. The Σ^α operators correspond to global π spin-rotations about the αth axis and with periodic boundary conditions we have $\Sigma^x\Sigma^y = (-1)^N \Sigma^z$ where N is the total number of sites.

With these definitions, we now state and prove the necessary and sufficient condition that the perturbation H_P *does not* change at least one dynamic spin-spin correlation (*i.e.* $(\langle\langle \sigma_r^\alpha(t)\sigma_0^\alpha(0)\rangle\rangle)$) from short ranged to a long ranged one (in power-law sense). The condition is:

$$[\Sigma^\alpha, H_P]_- = 0 \quad \forall\alpha, \tag{2}$$

where $[..]_{-(+)}$ denotes the commutator (anti-commutator). *If this condition is violated, then at least one component of the dynamical spin-spin correlation becomes a power law.* To prove this we take the case of $\langle\langle \sigma_r^z(t)\sigma_0^z(0)\rangle\rangle$ for concreteness (without loss of generality). We note that in terms of the Majorana Fermions we have $\sigma_i^\alpha = -ib_i^\alpha c_i$ [1–3]. Thus the operation of σ_i^α creates a c Fermion on the i^{th} site as well as two quanta of Z_2 flux on adjacent plaquettes which share an α-type bond. This is schematically illustrated in Fig. 2 (left panel). Thus the operators σ_r^α and σ_0^α create such fluxes centered around r and 0 respectively. Since the perturbation does not conserve flux, one can always repeatedly apply H_P and move the pair of flux centered at r to the pair centered at 0 and then annihilate them. This occurs at order $\sim r$ of the perturbation theory and one has a string of perturbation operators joining 0 and r. Such a process has a leading term $\lambda^r = e^{-r\ln(1/\lambda)}$ which gives rise to exponential decay of spin correlations with correlation length $\xi \sim 1/\ln(1/\lambda)$.

The above discussion indicates that in order to get long-ranged correlations, the perturbation term must neutralize the two pairs of fluxes centered at r and 0 locally and independently without forming the intermediate string whose length scales with r. This requires that the application of σ_i^α changes Σ^β for at least two values of β, *e.g.* $[\Sigma^{x(y)}, \sigma_i^z]_+ = 0$ and $[\Sigma^z, \sigma_i^z]_- = 0$. Thus the perturbing Hamiltonian, H_P, must be able to change the corresponding Σ^as in order to neutralize the flux locally. This is possible when the generic condition

$$[\Sigma^\beta, H_P]_+ = 0 \tag{3}$$

is fulfilled *for the corresponding two pair of βs*. Eqs. 2 (3) represents the necessary and sufficient conditions that a perturbing Hamiltonian H_P does not (does) change the nature of the spin correlators.

To illustrate these conditions via specific examples, we consider $H_p = H_z$ (studied in Ref. [8]). It is easy to see that $[\sigma_r^z, \Sigma^{x(y)}]_+ = 0$ and $[\sigma_r^z, \Sigma^z]_- = 0$. Thus the Z_2 fluxes are neutralized locally leading to long-ranged spin correlators. For a Zeeman term in the z direction, only the zz correlators become power-law while xx or yy correlators remain exponential as before. The above results hold for $H_P = H_b$ when $\alpha \neq \beta$. Next, we consider $H_P = H_h$. The individual terms in H_h are of the form $\sigma_i^\alpha \sigma_j^\alpha$, where i and j are nearest neighbors. If $\langle ij \rangle$ is in the α^{th} direction, they commute with all W_p. Otherwise,

each spin operator flips two distinct pairs of W_ps on the plaquettes which share the bond $i, i+e_a$ and $j, j+e_a$. However, it is easy to check that Σ^α contains either both or none of the flipped W_ps and hence H_h commutes with all the three Σ^α. H_h therefore fails to destroy the short ranged nature of the spin-spin correlations.

Having established the general setting, let us now look at the spin-spin correlation in detail. A typical $n^{\rm th}$ order term in the perturbation expansion for the spin-spin correlation is, $T_n = \sum_{\langle i_1 j_1\rangle}\cdots\sum_{\langle i_n j_n\rangle}\int d\tau_1\cdots\int d\tau_n \langle \mathcal{T}\Big(\sigma_r^\alpha(\tau) h_{i_1 j_1}^{a_1}(\tau_1) h_{i_2 j_2}^{a_2}(\tau_2) ... h_{i_n j_n}(\tau_n)\sigma_0^\alpha(0)\Big)\rangle/n!$, where h_{ij}^a stand for the individual terms in H_P. Here we have taken all operators to evolve in Euclidean time, $O(\tau) = e^{H_K \tau} O e^{-H_K \tau}$. Consider now the case when r is sufficiently far from the origin. At any finite order, n (with n being even) T_n may be written as $T_n = \sum_{\langle i_1 j_1\rangle}\cdots\sum_{\langle i_n j_n\rangle}\int d\tau_1\cdots\int d\tau_n \langle \mathcal{T}\Big([\sigma_r^\alpha(\tau) h_{i_1 j_1}^{a_1}(\tau_1) h_{i_2 j_2}^{a_2}(\tau_2) ...]\,[\cdots h_{i_n j_n}(\tau_n)\sigma_0^\alpha(0)]\Big)\rangle/n!$, where we have divided up the series using $[\cdots]$ such that the fluxes are neutralized around r and 0 respectively by the operators belonging to each group within the square brackets. Once the fluxes are neutralized, the b_i^α Fermions are no longer important except for an overall constant. The c Fermions now determine the details of the correlation. In the gapless phase of the Kitaev model the c fermions have a Fermi-surface and gapless excitations across it. Thus the c-Fermion propagator is an $n^{\rm th}$ order free Fermion propagator, which in $(2+1)$ dimension, is given by $\mathcal{G}_c(\beta, r, \tau) \sim \left(r^2+\tau^2\right)^{-(np/2+1)}$, where p is the number of σ operators occurring in h_{ij}^a. Thus we expect that the connected spin-spin correlation function goes as:

$$\langle\langle \sigma_r^\alpha(t)\sigma_0^\alpha(0)\rangle\rangle \sim \lambda^n \left(r^2-t^2\right)^{-(np/2+1)}, \qquad (4)$$

where λ is the coupling constant. Eq. 4 reproduces the results of Ref. [8] where $p=1$ and $n=2$.

We note that the above results are valid for infinite 2D systems and our conclusion may change for finite systems such as nanotubes, *i.e.*, a cylinder of infinite length and (finite) perimeter L. In this case it may be possible to annihilate the Z_2 flux locally by going around the finite direction of the cylinder even for a perturbation which does not induce power-law correlations in an infinite system. This leads to a crossover of the behavior in the correlation function. For $L \gg r$, it is easier to construct the string joining 0 and r (at the lower order of perturbation theory) than going around the cylinder and the infinite geometry results hold. However, for $r \ll L$, it is easier to form a string round the axis of the cylinder annihilation of the Z_2 flux leading to to power-law correlators. Such a term occurs at order $\sim \lambda^L$ of the perturbation theory.

Next, we study the phase diagram of the Kitaev model augmented by a loop term $H_L = -\kappa\sum_p W_p$ and perturbed by an Ising-like perturbation $H_I = \lambda\sum_{\langle ij\rangle} S_i^z S_j^z$ for $J_{1,2,3}=1$ and within a RVB mean-field theory. To this end, we use our earlier transformation $\sigma_i^\alpha = -ib_i^\alpha c_i$ to map the spin model $H_K+H_L+H_I$ to a Fermionic model H_F. The resultant Hamiltonian becomes

$$\begin{aligned} H_F &= -\sum_{j\in A}\Big[\sum_{\alpha=x,y\,links} ic_j c_{j'_\alpha} + \sum_{z\,link} ib_j^z c_j ib_{j'_z}^z c_{j'_z}\Big] \\ &\quad -\kappa \sum_{j,k\in plaquette}\sum_{zlink} ib_j^z b_{j'_z}^z ib_k^z b_{k'_z}^z \\ &\quad +\lambda\sum_j \sum_{\alpha=all\,links} ib_j^z c_j ib_{j'_\alpha}^z c_{j'_\alpha}, \end{aligned} \qquad (5)$$

where the subscript $j,k \in plaquette$ indicates that the sum is over sites which belong to the A sublattice of a given plaquette as schematically shown in Fig. 1. Note that for $\lambda=0$, the operators $ib_j^z b_{j'_z}^z$, commute with the Hamiltonian and are therefore a constants of motion. In this limit, H is exactly solvable. When λ is turned on, these operators acquire dynamics and their fluctuations are ultimately expected to confine the spinons through a confinement-deconfinement transition.

To make further progress, we introduce RVB type mean-fields [3, 4] on the sites (corresponding to spin ordering) and on links (corresponding to the emergent gauge fields) of the hexagonal lattice: $\langle ib_j^z c_j\rangle = \langle\sigma_j^z\rangle = \Delta_{1(2)}$, $\langle ib_j^z c_{j'_\alpha}\rangle = \beta_\alpha$, $\langle ib_j^z b_{j'_\alpha}^z\rangle = \gamma_\alpha$, and $\langle ic_j c_{j'_\alpha}\rangle = \gamma_{0\alpha}$. Note that keeping in mind the bipartite nature of the hexagonal lattice and to allow for possible AFM phases, we have introduced two mean-fields Δ_1 and Δ_2 corresponding to the two sublattices shown in Fig. 1. Decomposing the quartic term in H_F in using these mean fields we have the quadratic mean-field Hamiltonian, which, in momentum space, is given by

$$\begin{aligned} H_{\rm mf} &= \frac{1}{N}\sum_{\vec k}\Big[J_0\left(\alpha + e^{ik_1} + e^{i(k_1+k_2)}\right) c_{\vec k}^{A\dagger} c_{\vec k}^B \\ &\quad + J_0^{'}\left(\beta - 2\kappa\gamma_z/J_0^{'} + e^{ik_1} + e^{i(k_1+k_2)}\right) b_{\vec k}^{A\dagger} b_{\vec k}^B \\ &\quad + (ic_{\vec k}^{A\dagger} b_{\vec k}^B - ib_{\vec k}^{A\dagger} c_{\vec k}^B)\left(\beta_z(1+\lambda) + \beta_x e^{ik_1}\right. \\ &\quad \left. + \beta_y e^{ik_2}\right) - c_1 b_{\vec k}^{A\dagger} c_{\vec k}^A - c_2 b_{\vec k}^{B\dagger} c_{\vec k}^B + {\rm h.c}\Big] \\ &\quad + \kappa\gamma_z^2 - (1+\lambda)\gamma_z\gamma_{0z} + (1+3\lambda)\Delta_1\Delta_2, \end{aligned} \qquad (6)$$

where $J_0 = (1+\lambda\gamma_x)$, $\alpha J_0 = (1+\lambda)\,\gamma_z$, $J_0^{'} = \lambda\gamma_{0x}$, $\beta J_0^{'} = (1+\lambda)\,\gamma_{0z}$, $c_{1(2)} = (1+3\lambda)\Delta_{1(2)}$, and the momentum $\vec k = k_1\hat e_1 + k_2\hat e_2$ with the unit vectors $\hat e_1 = \hat x + \hat y/\sqrt{3}$ and $\hat e_2 = 2\hat y/\sqrt{3}$.

We now minimize $H_{\rm mf}$ numerically and obtain the mean-field phase diagram of the model as a function of λ and κ. Note that the mean field solution is exact at $\lambda=0$. This phase diagram is shown in the left panel of Fig. 3. In accordance with our expectation, we find that at large positive (negative) λ, the ground state of the model is an Ising AFM (FM) which corresponds to

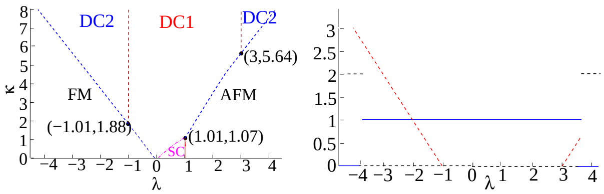

FIG. 3: (Color online) Left Panel: The mean-field phase diagram for the model. The blue dashed lines represent confinement-deconfinement transitions. The triple points occur at $(\lambda_1^*, \kappa_1^*) = (1.01, 1.07)$ and $(\lambda_2^*, \kappa_2^*) = (3, 5.64)$ for $\lambda > 0$ and $(\lambda_3^*, \kappa_3^*) = (-1.01, 1.88)$ for $\lambda < 0$. Right Panel: Plot of the loop order parameter (solid blue line), the spinon gap (red dashed line) and the FM and the AFM order parameters (black dashed lines) as a function of λ for $\kappa = 7$.

confined phase of spinons while at small λ, the model exhibits a deconfined gapless phase DC1. The transition between DC1 and AFM , at low κ and positive λ, occurs via a intermediate SC phase, which corresponds to antiferromagnetic alignment of spins along chains in x direction of the hexagonal lattice with ferromagnetic arrangement of such chains in the y direction. For negative λ, there is a direct transition to the FM phase from DC1 (for small κ). At high enough values of κ, we find another gapped deconfined phase DC2. The transition between DC1 and DC2 is and second order within mean field theory and is an example of a topological quantum phase transition. The confinement-deconfinement transitions at high κ always occur from DC2 to AFM/FM phases. These transitions are predicted to be first order within mean-field theory. The phase diagram exhibits two triple points at $(\lambda_1^*, \kappa_1^*) = (1.01, 1.07)$ and $(\lambda_2^*, \kappa_2^*) = (3, 5.64)$ for $\lambda > 0$. These represent meeting points of AFM, SC and DC1 and AFM, DC2 and DC1 phases respectively. For $\lambda < 0$, there is one triple point $(\lambda_3^*, \kappa_3^*) = (-1.01, 1.88)$ where the FM, DC1, and DC2 phases meet. We also note that our mean-field analysis also gives an estimate for the stability of the deconfined phase of the Kitaev model ($-0.07 \leq \lambda_c \leq 0.08$ for $\kappa = 0$) under external perturbing Ising term which may be important for physical realization of the Kitaev model and for quantum computing proposals based on it [5, 7].

The plot of the loop order parameter $\langle W_p \rangle$, the spinon gap, and the AFM and the FM order parameters as obtained from the mean-field theory, is shown, for $\kappa = 7$, as a function of λ in the right panel Fig. 3. We note that all the order parameters show discontinuous changes at the transition points indicating first order transitions. The spinon gap, in contrast, increases linearly and continually with λ indicating a second order quantum phase transition between DC1 and DC2 phases. The presence of this topological quantum phase transition and the linear variation of the spinon gap with λ can be understood qualitatively from $H_{\rm mf}$. For large κ, it requires a large λ to destabilize the Kitaev ground state in favor of Ising AFM/FM. In addition, numerically we find that in the Kitaev phase $\gamma_z(\gamma_x) \sim 1(0)$. As a result, beyond a critical value of $\lambda = \lambda_c$, the effective couplings along the links, $J_{1,2} \sim (1 + \lambda\gamma_x)$, $J_3 \sim \gamma_z(1 + \lambda)$, fail to satisfy $|J_1 - J_2| \leq J_3 \leq J_1 + J_2$ thus leading to a gapped phase via a topological quantum phase transition [1, 2]. The spinon gap in this gapped phase varies linearly with J_3 [2, 3] and hence shows a linear variation on λ. At small κ, the confinement-deconfinement transitions to the SC/FM phases occur before λ_c is reached and hence the topological phase transitions do not occur.

To conclude, we have presented a general classification of the contaminating interactions of the Kitaev model based on their effects on the spin correlators of the model and have derived a necessary and sufficient condition for the interaction to induce power-law spin-spin correlations. We have also presented the phase diagram of the Kitaev model, augmented by a loop term and perturbed by an Ising Hamiltonian, and have shown that the model exhibits a rich phase diagram with several interesting transitions. Our estimate suggests that the topological phase of the Kitaev model is unstable to about 10% contamination by Ising interactions.

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